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PHYSICS OF PLANETARY ATMOSPHERES I: RAYLEIGH SCATTERING BY HELIUM

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RAYLEIGH SCATTERING BY HELIUM

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ABSTRACT

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A variational method is used to calculate the Rayleigh scattering cross sections of helium as a function of wavelength. The value at Lyman-α is 3.53×10^{-26} cm^2.

Author

INTRODUCTION

The cross section for the scattering of light by an atomic gas may be obtained from the refractive index.

The refractive index of helium has been measured with high precision at wavelengths between 2700Å and 5400Å [1]* and the measurements can be extrapolated to longer wavelengths without serious loss of accuracy. The extrapolation to shorter wavelengths has been carried out using a semi-empirical procedure [2], but the accuracy is uncertain. The refractive index can be calculated directly at any wavelength by variational procedures similar to those employed in the calculation of static polarizabilities and with comparable accuracy.

Our procedure, which relates the evaluation of infinite summations to the solutions of differential equations, differs in its approach from those discussed by Karplus et al. [3-7].

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* Numbers in [ ] throughout the text represent reference numbers.

THEORY

The refractive index n of a gas of number density N is given by

$$n - 1 = 2\pi N\alpha(\nu) \qquad (1)$$

where $\alpha(\nu)$ is the frequency-dependent atomic or molecular polarizability. If the atom or molecule is in a state with eigenfunction ψ_0 and ψ_s represents the eigenfunctions of the other quantum states

$$\alpha(\nu) = \frac{2}{3h} S' \frac{\nu_{s0}}{\nu_{s0}^2 - \nu^2} |(0|\underline{m}|s)|^2 \qquad (2)$$

where ν_{s0} is the eigenfrequency of the transition from ψ_0 to ψ_s and $\underline{m}$ is the electric dipole moment

$$\underline{m} = \sum_i e_i \underline{r}_i \qquad (3)$$

e_i being the charge of the $i\underline{th}$ particle and $\underline{r}_i$ being its position vector. The polarizability (2) can be written alternatively as

$$n - 1 = \frac{1}{3h} \underset{s}{S'} \left(\frac{1}{\nu_{s0}+\nu} + \frac{1}{\nu_{s0}-\nu}\right) |(0|\underline{m}|s)|^2 \qquad (4)$$

or as

$$n - 1 = \frac{1}{12\pi^2 m\nu^3} \underset{s}{S'} \left(\frac{1}{\nu_{s0}+\nu} - \frac{1}{\nu_{s0}-\nu}\right) (0|\underline{m}|s)(s|\underline{m}'|0) \qquad (5)$$

where $\underline{m}'$ is the electric gradient operator

$$\underline{m}' = \sum_i e_i \nabla_i \quad . \qquad (6)$$

Now introducing a function $X(\underline{r}_i/\nu)$ such that

$$(H - E_0 + h\nu)X(\nu) + \underline{m}\psi_0 = 0 \qquad (7)$$

where

$$(H - E_0)\psi_0 = 0 \qquad (8)$$

it may be shown (cf. Dalgarno [8,9]) that (4) is equivalent to

$$n - 1 = \frac{1}{3}[\{\chi(\nu) + \chi(-\nu)\}, \underline{\underline{m}}\psi_0] \tag{9}$$

and (5) to

$$n - 1 = \frac{h}{12\pi^2 m\nu^3} [\{\chi(\nu) - \chi(-\nu)\}, \underline{m}'\psi_0] \tag{10}$$

Equation (10) can be written alternatively as

$$n - 1 = \frac{h}{12\pi^2 m\nu^3} [\{\chi'(\nu) - \chi'(-\nu)\}, \underline{\underline{m}}\psi_0] \tag{11}$$

where

$$(H - E_0 + h\nu)\chi'(\nu) + \underline{m}'\psi_0 = 0. \tag{12}$$

Equation (7) may be solved by constructing a functional

$$J(\nu) = \{\chi(\nu)|H - E_0 + h\nu|\chi(\nu)\} + 2\{\chi(\nu), \underline{\underline{m}}\psi_0\} \tag{13}$$

and minimizing $J(\nu)$ with respect to some trial form of $\chi(\nu)$. Then

$$\alpha(\nu) = \frac{1}{3}\{J(\nu) + J(-\nu)\} \tag{14}$$

is a lower bound to the polarizability (provided ψ_0 is an exact eigenfunction of H).

CALCULATIONS

We adopted for the ground state of helium the 20-parameter representation of Hart and Herzberg [10] and a trial function $\chi_t(\nu)$ of the form

$$\chi_t(\nu) = \sum_{s=0}^{m} c_s(\nu)(\underline{r}_1 r_1^{\ s} + \underline{r}_2 r_2^{\ s})\psi_0(\underline{r}_1, \underline{r}_2) \tag{15}$$

the $c_s(\nu)$ being variational parameters. Substituted into (14) they yield a static polarizability ($\nu = 0$) of 0.204×10^{-24} cm^3 in close agreement with the most accurate value available: 0.205×10^{-24} cm^3 [11].

As Table 1 demonstrates, the convergence of $\alpha(\nu)$ as a function of the number of variational parameters is very rapid for the visible region of the spectrum but less so as the first resonance wavelength is approached. The proper change in the sign of $J(\nu)$ does occur as the wavelength is decreased, the first pole occurring at 573Å compared with the correct location of 584Å. Attempts to proceed to larger numbers of variational parameters led to serious numerical instabilities.

The values of $n - 1$ measured by Cuthbertson and Cuthbertson [1], which refer to wavelengths longer than 2750Å, exceed the predicted values by 0.44% near 9000Å, the excess increasing to 0.50% at 2750Å. We have accordingly increased the theoretical values uniformly by 0.47% and they are presented in Figures 1 and 2, which include also the measured values.

The cross section for the scattering of isotropic unpolarized radiation is given by

$$Q = \frac{128\pi^5}{3\lambda^4}\,\alpha(\nu)^2 \tag{16}$$

and values of Q may be readily derived from Figures 1 and 2.

The cross section for scattering of Lyman-α is 3.53×10^{-26} cm^2. Values for some other wavelengths are given in Table 2.

TABLE 1

Convergence of $\alpha(\nu)$

Wavelength (Å) \ m	0	1	2	3	4
9110	1.132	1.378	1.379	1.379	- 1.379
3037	1.147	1.413	1.414	1.414	1.414
911	1.319	1.905	1.950	1.952	1.952
759	1.422	2.307	2.452	2.465	2.467
607	1.661	3.869	5.507	6.342	6.786
569	1.775	5.288	13.18	56.86	- 38.61

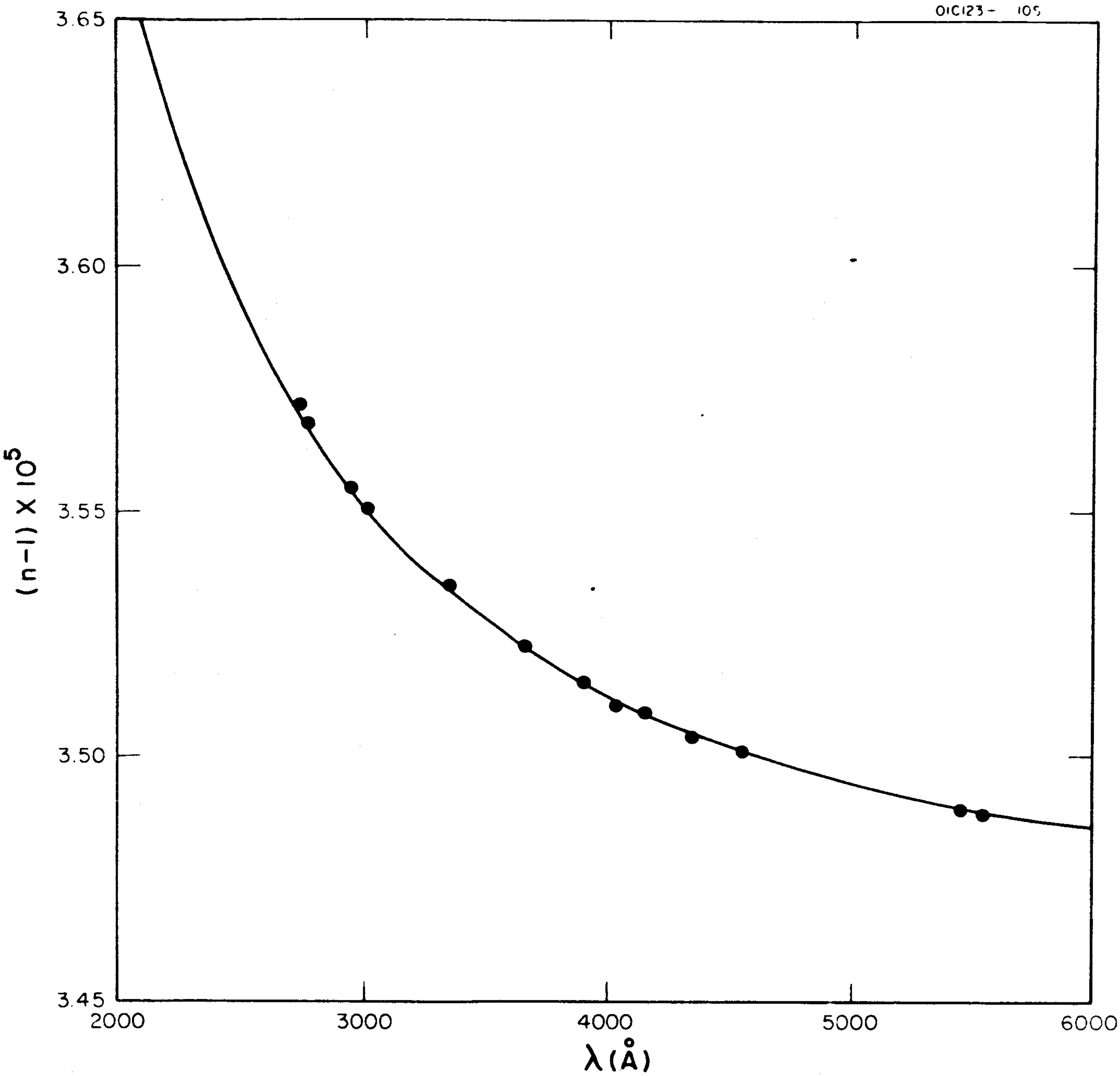

Figure 1. The refractive index of helium.

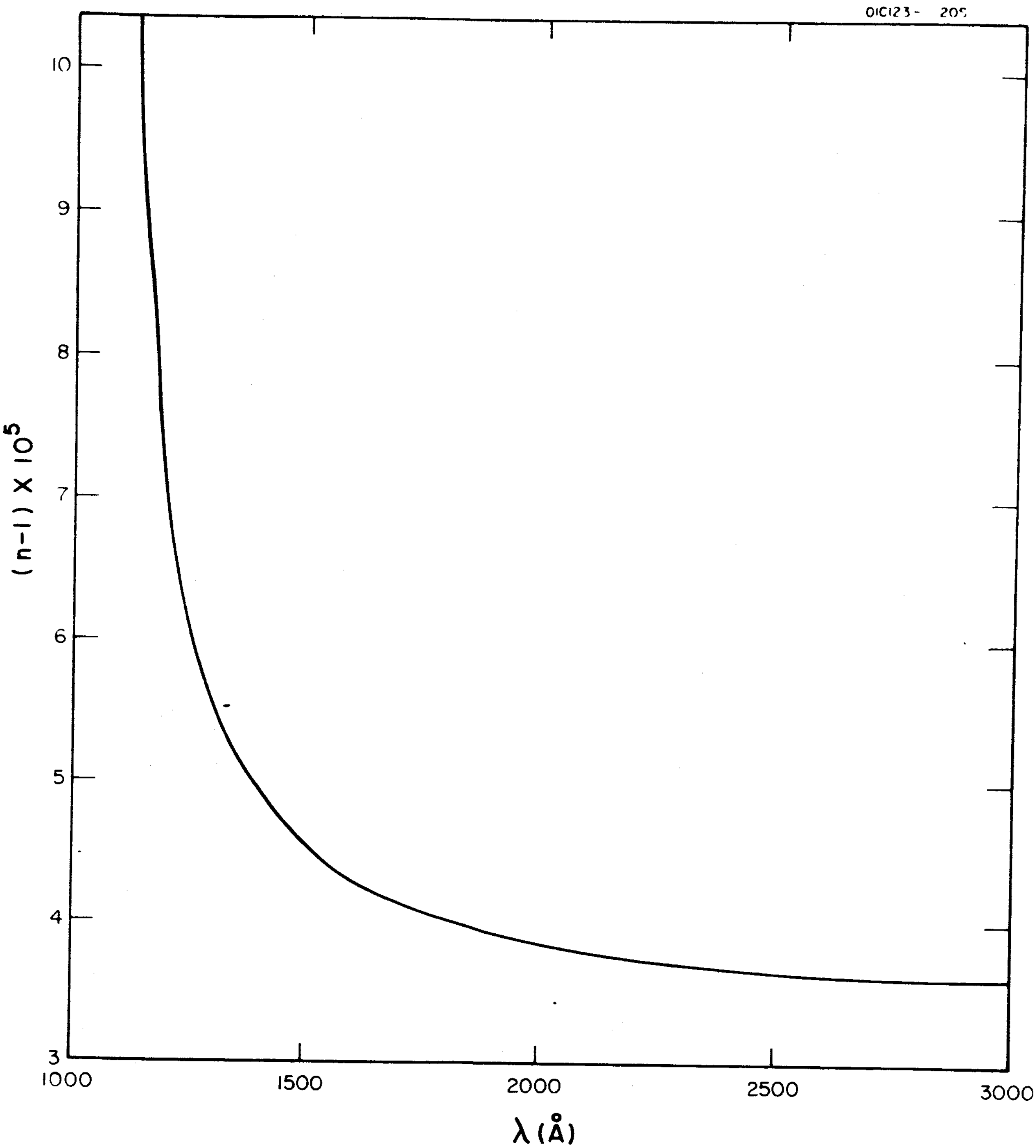

Figure 2. The refractive index of helium.

TABLE 2

Light Scattering Cross Sections Q cm^2

(Å)	700	800	1000	1500	2000	2500
Q(cm^2)	1.07×10^{-24}	3.56×10^{-25}	9.51×10^{-26}	1.33×10^{-26}	3.83×10^{-27}	1.50×10^{-27}

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